Phase diagrams of cuprate superconductors

i) Perspective on the phase diagram of cuprate high-temperature superconductors
Authors: D. Rybicki, M. Jurkutat, S. Reichardt, C. Kapusta, and J. Haase
arXiv:1511.02408 (Nature Communications **7**, Article number: 11413 (2016))

ii) Bulk superconductivity at 84 K in the strongly overdoped regime of cuprates
Authors: A. Gauzzi, Y. Klein, M. Nisula, M. Karppinen, P. K. Biswas, H. Saadaoui, E. Morenzoni, P. Manuel, D. Khalyavin, M. Marezio, and T. H. Geballe
arXiv:1612.04707 (Physical Review B **94**, 180509(R) (2016))

Recommended with a Commentary by Jörg Schmalian, Karlsruhe, Germany

If one performs a google-images search for *"phase diagram of cuprate superconductors",* one finds an impressive number of hits with rather similar plots, implying that this must be a settled issue. The plots all display transition- and crossover-temperatures as function of doping, x, with a rapidly dropping antiferromagnetic phase, a semicircular "dome" of superconductivity, strange metal behavior near optimal doping, and rich physics below the so-called pseudo-gap temperature. Given the chemical complexity of the cuprates, the success of such $T(x)$-plots is rather surprising. Undoubtedly, it has proven to be a powerful approach that allowed comparing and unifying cuprate superconductors. Theoretically manifested in single-orbital Hubbard[1] and t-J[2] models, the approach found early experimental support[3]. In Ref.[3] Takigwa *et al.* showed that NMR Knight-shifts of oxygen and copper nuclei (measuring the spin-susceptibility projected onto states with orbital wave function, dominated by oxygen and copper states, respectively) have similar temperature dependencies. This led to the widely accepted view of a single-spin fluid in the cuprates, as expected from a single-orbital description.

The recent analysis by Rybicki *et al.* concludes that a more detailed analysis is needed i) to understand the significant variations amongst the different classes of cuprate superconductors and ii) to find ways to increase the superconducting transition temperature T_c of the cuprates. The authors propose a higher-dimensional phase diagram that plots T_c as function of the doped holes in oxygen (n_p) and copper (n_d) orbitals: $1+x = n_d + 2n_p$. The individual hole-counts are obtained from measurements of the NQR quadrupolar shifts $^{17}\nu_Q$ and $^{63}\upsilon_Q$, well known to be sensitive to n_p and n_d, respectively. In fact those shifts are frequently used to place a material properly in the $T(x)$ phase diagram. The key observation of Rybicki *et*

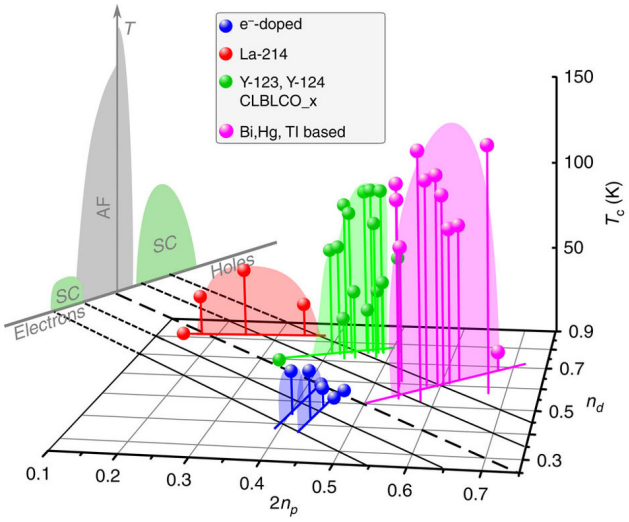

FIG. 1: Superconducting transition temperature T_c as function of oxygen (n_p) and copper (n_d) hole count. The plot suggests that charge transfer to the oxygen orbitals leads, for fixed total hole count $x = 2n_p + n_d$, to higher T_c (figure taken from Rybicki *et al.* Nature Comm. **7**, 11413 (2016)).

al. is the higher-dimensional phase diagram of Fig.1. This figure strongly suggests that, for fixed x, systems with larger n_p, i.e with more transferred holes in the planar oxygen states, give rise to larger transition temperatures. Rybicki *et al.* further find a correlation betw*een* T_c *and* n_p, reminiscent to the famous Uemura plot[5]. The authors therefore conclude that one should *"synthesize materials that lead to an increased planar oxygen hole content at the expense of that of planar copper".*[4] Of course, this is not the first attempt to develop a systematic analysis of different cuprate sub-families. Interlayer spacings, bond lengths, electronegativity, have all been analyzed and display clear correlations with T_c. The appeal of the conclusion of Rybicki *et al.* is that it convincingly relates T_c with a "reasonably microscopic" quantity. If combined with the impressive early analysis by Ohta, Tohyama, and Maekawa[5] one further concludes that parameters like the apical oxygen position and the c-axis bond length will essentially trigger this Cu-O charge transfer, which seems to be the primary knob to turn if one wants to increase T_c.

What do we learn from this analysis? Superconductivity in the cuprates sensitively depends on the balance between copper an oxygen electronic states. There are, at least, two theoretical scenarios that seem consistent with this finding. It could be that the copper-oxygen charge balance "only" affects high-energy chemistry in the sense that it only determines the parameters (coupling constants, Fermi velocities etc.) of a universal, low-energy,

single-band theory. Alternatively, these results could be of more fundamental importance and express the need of a multi-orbital description to properly formulate the high-T_c problem.

The traditional rule, according to which the total charge content determines the transition temperature, is also challenged in the recent paper by Gauzzi et al., who find $T_c = 84K$ in a materials that seems to be on the strongly overdoped side of the phase diagram. The authors investigate high-pressure oxidized $Cu_{0.75}Mo_{0.25}Sr_2YCu_2O_{7.54}$, in which overdoping is achieved up to $x \approx 0.45$, i.e well beyond the usual superconducting dome. This materials seems to be a natural candidate to check the proposal of Rybicki *et al.*. Unconventional behavior, even challenges to the view that overdoped systems can be described as Fermi liquids, have been made in Ref.[6,7] and in the findings by Rybicki *et al.*. One would also expect that the role of oxygen versus copper doping and thus, the differences between the above two theoretical scenarios, is most pronounced for large doping concentrations. This suggests to focus our attention to this inexcusably neglected part of the phase diagrams of the cuprates.

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[1] P. W. Anderson, Science **235**, 1196 (1987).

[2] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[3] M. Takigawa, A. P. Reyes, P. C. Hammel, J. D. Thompson, R. H. Heffner, Z. Fisk, and K. C. Ott Phys. Rev. B **43**, 247 (1991).

[4] Note, the analysis of Rybicki *et al.* is not in contradiction to the NMR-data that led to the single-spin fluid interpretation. Both can be reconciled if the corresponding Knight shifts contain different T-independent contributions.

[5] Y. Ohta, T. Tohyama, and S. Maekawa Phys. Rev. B **43**, 2968 (1991).

[6] Y. J. Uemura, *et al.*, Phys. Rev. Lett. **62**, 2317 (1989).

[7] I. Božović X. He, J. Wu, and A. T. Bollinger, Nature (London) **536**, 309 (2016).